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Nucleation and Propagation of Deformation Twin in Polysynthetically Twinned TiAl

L. G. Zhou[1], L. M. Hsiung[2], and Hanchen Huang[1]

Abstract Using molecular dynamics simulations, we have studied the deformation of polysynthetically twinned (PST) TiAl at room temperature with a bicrystal model. The simulation cell was pre-strained and thermodynamically relaxed to a criterion that all stress components of the simulation cell have gone to zeros; in this way no dislocations were pre-existed in γ-α_2 interfaces. A uniaxial compression was then applied along one 1/6<112] direction in the surface. The results show that under the compression, the interfacial dislocation pairs were prolifically generated due to the structural transformation of α_2-lamella. The gliding and agglomerating of these dislocations would finally cause the nucleation of deformation twins from the interface. This is suggested to be a new possible twinning mechanism in the dual phase TiAl alloy. The propagation of this deformation twin, or specifically, its interaction with γ-γ and γ-α_2 interfaces has been discussed. It shows that the α_2-lamella is intent to block the propagation of the deformation twin.

Keyword: TiAl, twin, dislocation, interface, molecular dynamics.

1 Introduction

TiAl intermetallic compounds and alloys have been a focus of intensive research, due to their supreme properties at elevated temperatures. In particular, they possess high specific strength, high stiffness, and excellent environmental resistance [Appel and Wagner (1998)] at high temperatures. In addition, their density is low. Consequently, TiAl compounds and alloys are primary candidates of the structural materials in the aerospace industry. A major drawback of the compounds is the lack of ductility and toughness at room temperature. Recent efforts have been focused on the development of dual phase alloys with a refined full lamellar microstructure [Hsiung et al. (2002)]. The two phases are γ-TiAl and α_2-Ti_3Al, plus additional alloying elements. Increased fracture toughness and creep resistance result from the refined lamellar structure [Liu et al. (1996, 1998); Morris and Lip (1997)]. A polysynthetically twinned (PST) crystal of TiAl contains only fine lamellae of γ-TiAl and α_2-Ti_3Al [Wegmann et al. (2000); Parthasarathy et al. (2000)]. Such PST crystal is sometimes referred as a single crystal, although it contains twin boundaries. Because of the lamellar structure, PST crystals are highly anisotropic in mechanical properties. When the loading direction is parallel or perpendicular to the lamellar interfaces, the yield strength is high but the ductility is low. In contrast, under other loading directions the yield strength is low but the ductility is high [Inui et al. (1992)]. This anisotropy is related to the preferred glide of dislocations along interfaces. It is, therefore, possible to design materials of controllable strength and ductility by orientational alignment of the lamellae. The optimal design is still a target of on-going efforts [Maruyama et al. (1997)].

One of the controlling factors in the optimization is the deformation twin. According to Farent et al (1993), deformation twins in γ-TiAl form as a result of coordinated glides of a/6<112] partial dislocations. Similar mechanisms have been observed in dual phase TiAl, and the dislocation nucleation at grain boundaries is correlated with the local stress concentration [Jin and Beiler (1995)]. The twins may coarsen when ledges nucleate and migrate along the twin boundaries [Kim and Maruyama (2003)]. Instead of grain boundaries, γ–α_2 interfaces host dislocations due to the mismatch of two phases. These dislocations dissociate into partials at the interface. The glissile partials, either collectively after pileup at the interface [Hsiung et al. (1997, 2002)] or individually [Zhang and Ye (2003)], propagate away from the interface, leading to twin formation in the matrix. These experimental observations have clearly demonstrated the twin formation, and correlated it with pre-existing dislocations at the interface. In terms of twinning mechanism, are pre-existing dislocations necessary for the twin formation? And, how do the twins propagate? In this paper, we address these two issues using molecular dynamics simulations.

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2 Methodology

The molecular dynamics simulations involve four crucial components: setup of the simulation cell, interatomic potential, control of thermodynamic variables, and analysis techniques. In the following, we elaborate these four components one by one.

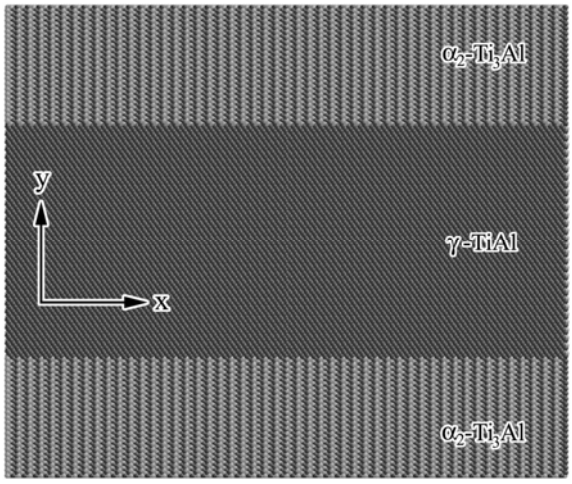


Figure 1: The simulation cell, with Ti atoms in light and Al atoms in dark spheres.

The simulation cell, shown in Figure 1, consists of two slabs, one being the γ-TiAl and the other α_2-Ti_3Al. The two slabs form an interface with both side being close-packed planes, that is $(111)_\gamma//(0001)_{\alpha 2}$. Further, the closed-packed directions on the two sides coincide with each other, that is $<110]_\gamma//<11\bar{2}0>_{\alpha 2}$ [Feng et al. (1989)]. The x-axis is along the $[\bar{1}12]_\gamma//[1\bar{1}00]_{\alpha 2}$, the y-axis the $[1\bar{1}1]_\gamma$ $//[0001]_{\alpha 2}$, and the **z** the $[110]_\gamma/[11\bar{2}0]_{\alpha 2}$. Periodic boundary conditions are applied along all the three directions. The intrinsic mismatches, 2.3% along **x** and 1.5% along **z**, and the corresponding stresses are relaxed through the control of thermodynamic variables; this will be elaborate after the description of interatomic potential. The dimensions of the simulation cell are 50.4 nm along x, 42.5 nm along y, and 2.3 nm along z; the total number of atoms is 288,000.

Atoms in the simulation cell interact with each other according to a prescribed interatomic potential. The Embedded Atom Method (EAM) potential of Ti-Al [Zope and Mishin (2003)] well describes the stability of multiple Ti-Al phases, and is used in this work.

With the prescribed interatomic potentials, atoms move according to the Newton's equation, under given stresses and temperatures. According to the Parrinello-Rahman algorithm [Parrinello and Rahman (1981)], the size and shape of a simulation cell respond to the difference of internal and external stresses, so the internal stresses are kept at desired values. We use this algorithm to control the stress in this work. The temperature of the simulation cell is essentially the kinetic energy. We scale the atomic velocities to control the temperature. In contrast to the use of frictional forces, the scaling scheme minimizes potential artificial impacts to defect activities.

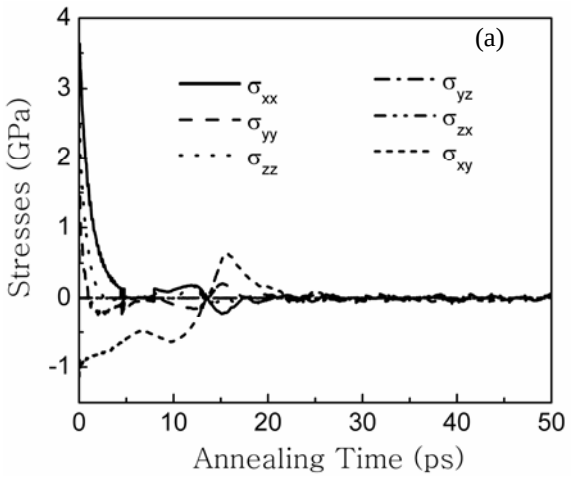
Under given stresses and temperatures, the molecular dynamics simulations provide details of atomic positions as a function of time. These positions must be analyzed to gain physical insights. The bond-pair analysis technique [Clarke and Jonsson (1993)] provides clear distinction between atoms in perfect crystals, interfaces, and near dislocations; and it is used in this study. According to this technique, a bond is considered to be formed between two nearest neighboring atoms. The configuration of others bonds formed by the nearest neighbors of the two atoms forming the bond determines whether the bond is good or bad. For example, each bond in a perfect face-centered-cubic (FCC) crystal has four neighboring bonds. Further, atoms in these four bonds form two other bonds. These two bonds form two non-connect chains, each being one bond in length. This bond configuration is referred to as "421". In the same logic, both 421 and 422 bonds form in hexagonal-close-packed (HCP) crystals. Near a stacking fault two layers of atoms are HCP-like, at a twin only one layer of atoms are HCP-like. In this work, the γ-phase is close to FCC, and the α_2-phase to HCP, and therefore the bond-pair analysis techniques applies.

3 Results

In this section, we present the mechanisms of twin nucleation and propagation in two-phase lamellar Ti-Al compounds, under mechanical loading. Before applying strains, we prepare an interface that is dislocation free.

Large mismatches exist in the initial simulation cell, shown in Figure 1. Using the Parrinello-Rahman algorithm, we relax the internal stress to zero. As shown in Figure 2a, all stress components of the simulation cell go to zeros beyond 25 ps. At the end of the relaxation, a twin is formed in the γ phase, as shown in Figure 2b. Incidentally, this newly formed twin enables the study of twin interactions, to be presented later.

Subjected to a uniaxial strain along x, applied at the rate of $2x10^8$ s^{-1} (that is $2x10^{-7}$ per molecular dynamics step), the atomic configurations in Figure 2b evolve. At 9.3 ps after the loading starts, pairs of interface dislocations nucleate at the γ-α_2 interface, as shown in Figure 3a. The dislocation nucleation enables interface migration (Figure 3b), which is driven by the strain imbalance. Before the loading, the γ phase is under tension, and the α_2 phase under compression. The compressive loading compensates the tension in the γ phase and reduces the strain energy, and its effect in the α_2



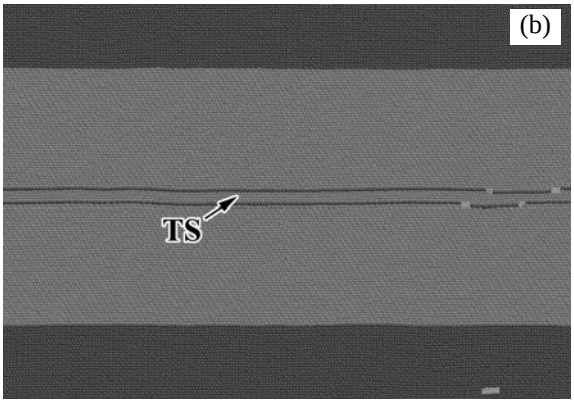
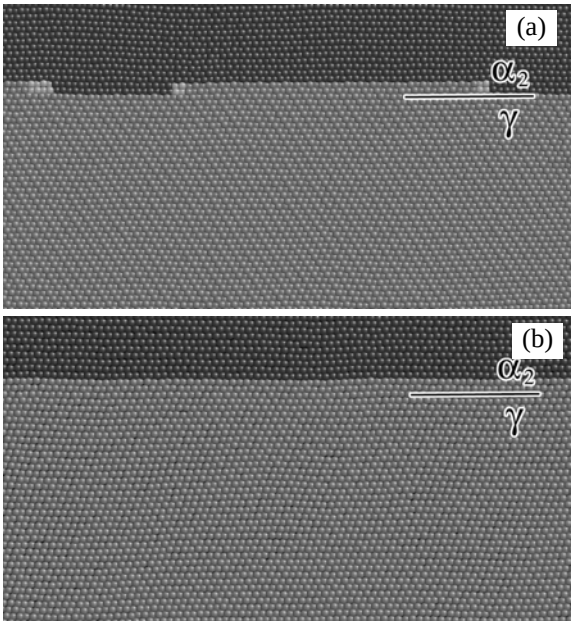


Figure 2: (a) Stresses during relaxation at 300K, and (b) relaxed atomic configuration (projection on x-y plane). The dark, dark gray, and light gray spheres represent HCP atoms, FCC atoms, and other atoms, respectively.



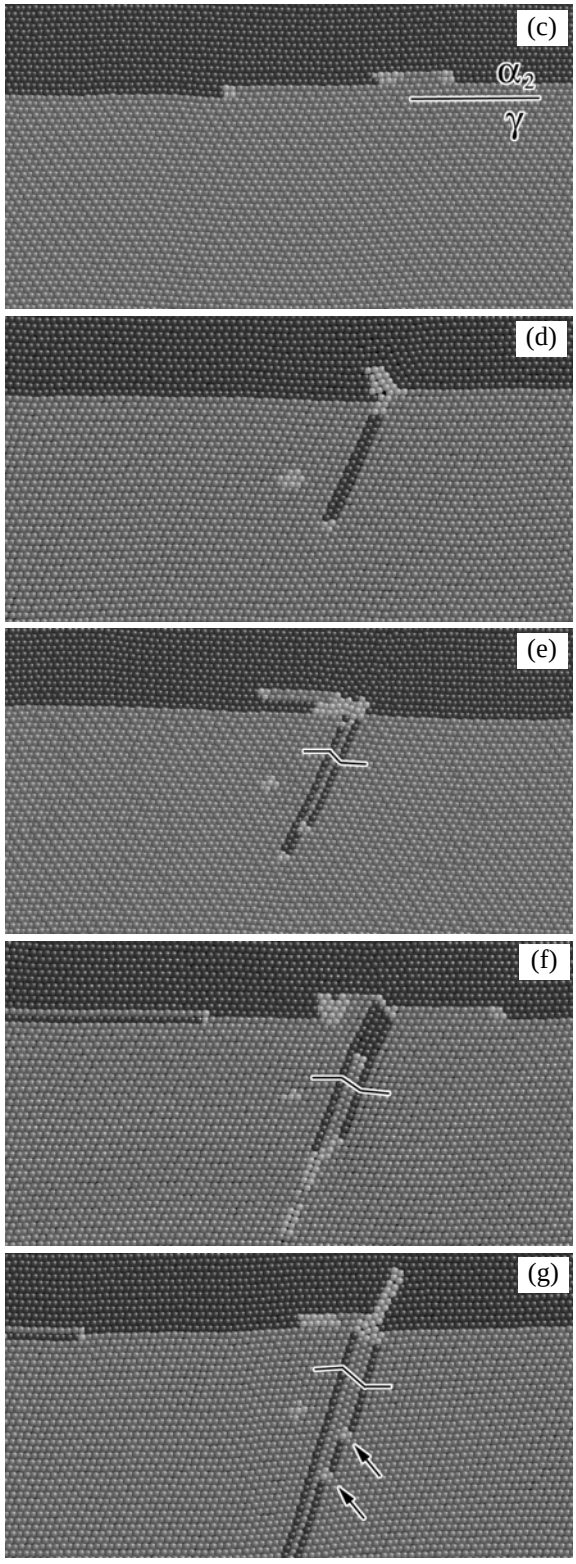
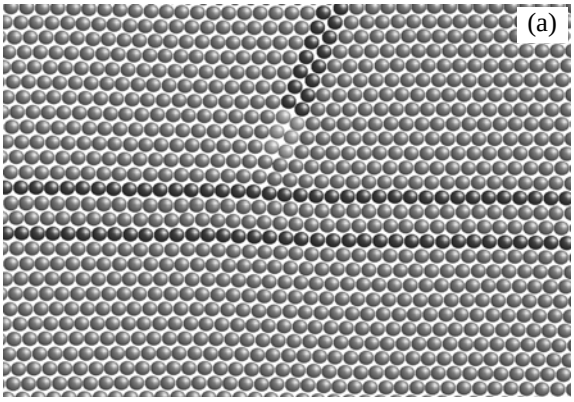


Figure 3: Twin emission from γ-α_2 interface. The dark, dark gray, and light gray spheres represent HCP atoms, FCC atoms, and other atoms, respectively.

phase is the opposite. Consequently, the γ-α_2 interface migrates into the α_2 phase, to reduce the strain energy. The motion of the interface forces the Ti_3Al atoms to arrange in the TiAl structure, and thereby increases the structure energy. The competition of the strain energy reduction and the structure energy increase eventually leads to stabilization of the interface. As shown in Figure 3c, some parts of the interface migrate toward α_2 and others toward γ phase. It is interesting to note that the two neighboring dislocations of the same sign agglomerate. It is worth to point out that, segments advancing into the α_2 lamella have the FCC stacking order and are not the γ phase. The thickness of this dislocation core (the step in the interface) is two atomic layers, consistent with the experimental observation of Hsiung et al (1997). This agglomeration leads to local stress concentration, which in turn triggers dislocation emission into the matrix. Glide systems of large Schmid's factor are readily available on the γ side. Indeed, one part of an interface dislocation emits into the γ phase, as shown in Figure 3d. Taking the γ phase structure as a reference, the interface dislocations have Burgers vectors of $1/6[\bar{1}12]$. The emitted dislocation has a Burgers vector of $1/6[1\bar{1}2]$, which comes from the following dislocation dissociation: $1/6[\bar{1}12] \rightarrow 1/6[1\bar{1}2] + 1/3[\bar{1}10]$. As the loading continues, another $1/6[1\bar{1}2]$ dislocation glides on $(1\bar{1}\bar{1})$ with the same mechanism, forming a nucleus of twin (Figure 3e). Once the twin has nucleated, the dislocation component left at the grain boundary is hard to move, as such it blocks the gliding of the other $1/6[\bar{1}12]$ (or $1/6[1\bar{1}2]$) interfacial dislocations (Figure 3f). This causes a larger localized stress, and therefore, the twin keeps growing by the successive emission of $1/6[1\bar{1}2]$, as pointed by arrows in Figure 3g.

So far our results have shown that a dislocation free γ-α_2 interface may emit twins. The emission happens by nucleation of dislocation pairs at the interface, and subsequent emission of partial dislocations from interface to the matrix. Continuation of the dynamic loading leads to propagation of the twin across another twin and a γ-α_2 interface.



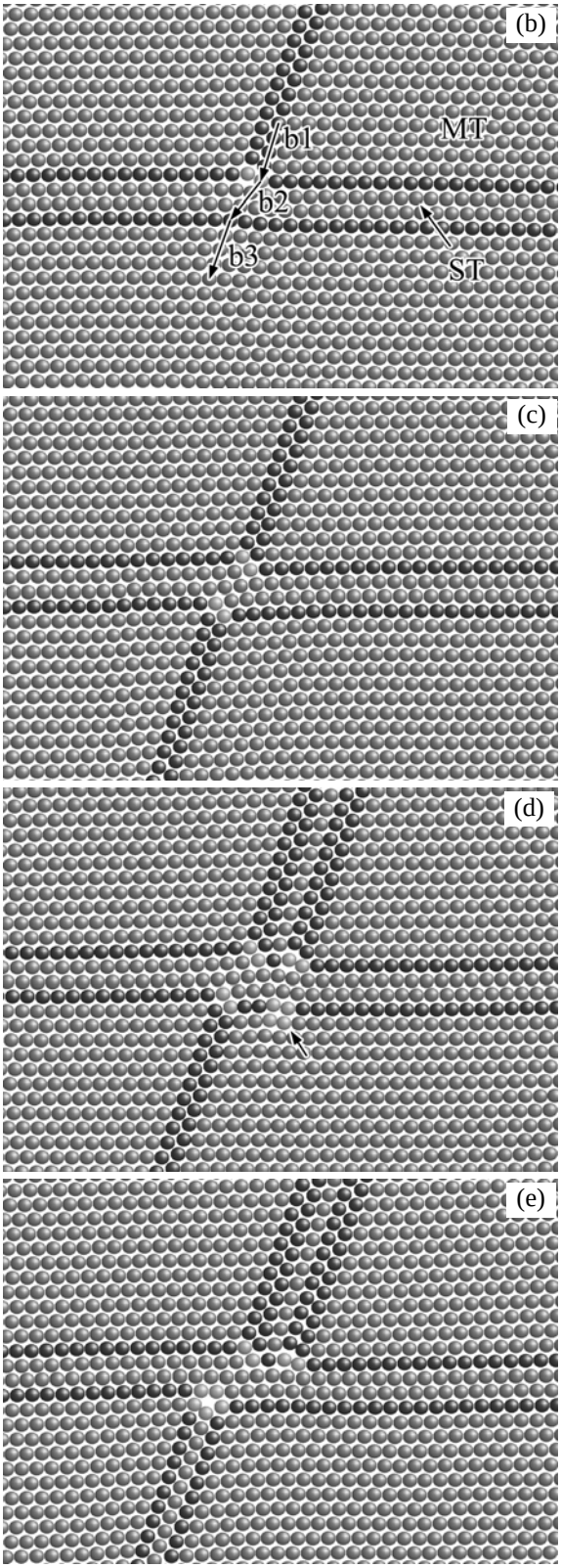


Figure 4: Twin (and partial dislocations) propagation cross a pre-existing twin.

As the load reaches 3.3% compressive strain, the emitted twin propagates toward a pre-existing twin, as shown in Figure 4a. A $1/6[1\bar{1}2]$ partial dislocation leads the propagation of the twin, and it glides on the $(1\bar{1}\bar{1})$ plane. An expanded view of the leading dislocation is shown in Figure 4b. The pre-existing twin ST forms during the initial structure relaxation, and now serves to interact with the newly emitted twin (and the leading partial dislocation). At the twin boundary, the partial dislocation $1/6[1\bar{1}2]$ dissociates into two dislocations $1/6[1\bar{1}4]$ + $1/3[00\bar{1}]$. The second dislocation, with Burgers vector **b2**=$1/6[1\bar{1}4]$, or $1/2[1\bar{1}0]$ in terms of the matrix ST, propagates across the twin (Figure 4b). At the following twin boundary, this dislocation **b2** =$1/6[1\bar{1}4]$ dissociates into two other dislocations, reversely: $1/6[1\bar{1}2]$ + $1/3[001]$. The dislocation, with Burgers vector **b3** = $1/6[1\bar{1}2]$, continues propagating. Crossing the twin, the leading partial dislocation has left behind two dislocations with Burgers vectors $1/3[00\bar{1}]$ and $1/3[001]$ (Figure 4c).

Following the leading partial dislocation is another one that borders the emitted twin. The second partial follows the footstep of the first, and forms a new twin, after passing through the pre-existing twin (Figure 4d). It is cautioned that the quantitative behavior of the second dislocation depends on the thickness of the pre-existing twins, in particular when two $1/6[1\bar{1}2]$ dislocations approach instead of repelling each other (Figure 4e). Therefore, we emphasize the mechanism of first dislocation passing through the pre-existing twin.

n contrast to the easy penetration of a twin boundary, a γ-α_2 interface is more difficult for the twin (and partial dislocations) to propagate across. As the strain reaches 3.5% compression, the partial propagating twin reaches the γ-α_2 interface, shown in Figure 5a. An expanded view near the interface is shown in Figure 5b. The twin is unable to propagate all together across the γ-α_2 interface. Instead, one partial dislocation is bounced back, while another one propagates through. At the interface, the propagating dislocation dissociates into two others according to the following Burgers vector balance: $1/6[1\bar{1}2] \rightarrow 1/24[5\ \bar{5}\ 14]$ + $1/24[\bar{1}1\bar{6}]$. The dislocation $1/24[5\ \bar{5}\ 14]$, or $[1\bar{1}02]/4$ in terms of the α_2 matrix, continues propagating into the α_2 phase, while the other dislocation $1/24[\bar{1}1\bar{6}]$ remains at the interface (Figure 5c). Upon the propagation of the leading partial dislocation, the other partial dislocation in the propagating twin also returns to the interface (Figure 5d). However, the front of the leading partial dislocation stops propagating forward into the α_2 phase. Instead, the front dislocation dissociates into two other dislocations, one going back toward the interface, and another parallel to the interface. This branching of the propagation ends the forward propagation of the leading partial dislocation and thereby the propagating twin.

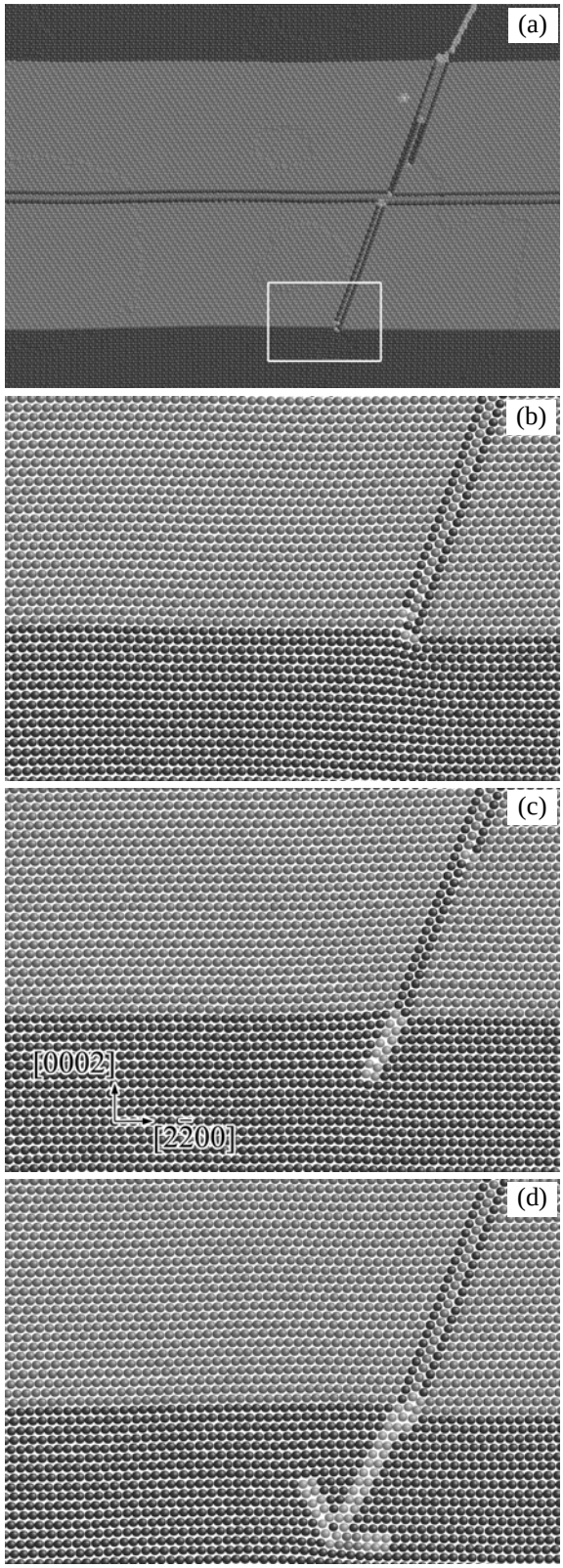


Figure 5: Interaction of the twin with γ/α_2 interface

The results of twin propagation show that it can easily go through another twin in the γ phase, leaving a $1/3[00\bar{1}]$ dislocation at each twin boundary. In contrast, the twin propagation across γ-$\alpha_2$phase is more difficult. This difficulty could lead to potential hardening effects.

4 Summary

Molecular dynamics simulations have been performed to study the interface deformation of PST TiAl. The results show that:

(1) The structural transformation taken place in the γ/α_2 interface, and therefore the generation of interface dislocations is the another factor except from the dislocation mismatch, that can cause the nucleation and propagation of the deformation twin from the γ/α_2 interface;

(2) Pioneered by a stacking fault crossing over the twin, the type I twin-twin interaction can be happened by the procedures of getting incident 1/6<112] dislocations from one side, then nucleating and growing a twin on the other side.

(3) The incident dislocation from the γ lamella is hard to propagate in the α_2 lamellas. Therefore the α_2 lamellas maybe lead to potential hardening effects.

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